

The Pessimistic Limits of Margin-based Losses in Semi-supervised Learning

Jesse H. Krijthe and Marco Loog

Abstract. We show that for linear classifiers defined by convex margin-based surrogate losses that are monotonically decreasing, it is impossible to construct *any* semi-supervised approach that is able to guarantee an improvement over the supervised classifier measured by this surrogate loss. For non-monotonically decreasing loss functions, we demonstrate safe improvements *are* possible.

Key words and phrases: Semi-supervised Learning, Margin-based loss, Surrogate loss, Logistic Loss, Hinge Loss, Quadratic Loss, Absolute Loss.

1. INTRODUCTION

Semi-supervised learning has delivered encouraging results in various settings, e.g. for object detection in computer vision [1], protein function prediction from sequence data [2] or prediction of cancer recurrence [3] in the biomedical domain and part-of-speech tagging in natural language processing [4]. In other settings, however, using unlabeled data has been shown to lead to a decrease in performance when compared to the supervised solution [4, 5]. For semi-supervised classifiers to be used safely in practice, we may at least want some guarantee that they improve performance over their supervised alternatives. Some have attempted to provide such guarantees either empirically by restrictions on the parameters to be estimated [6] or under particular assumptions on the data [7]. In general, however, it is unclear for what classifiers one can construct ‘safe’ semi-supervised approaches that can be expected to not decrease performance, or whether this is at all possible.

This work is concerned with the limits of the applicability of pessimistic semi-supervised classification. We wonder whether and, if so, how we can guarantee unlabeled data to improve a semi-supervised classifier in comparison to a supervised classifier. As our definition of such a ‘safe’ performance improvement, we consider the empirical surrogate loss a classifier typically optimizes and compare this loss for the supervised and the semi-supervised learner on the combined labeled and unlabeled data.

J.H. Krijthe is with the Department of Molecular Epidemiology, Leiden University Medical Center, Leiden, The Netherlands and the Pattern Recognition Laboratory, Delft University of Technology, Delft, The Netherlands. (e-mail: jkrijthe@gmail.com).
M. Loog is with the Pattern Recognition Laboratory, Delft University of Technology, Delft, The Netherlands and the Image Section, University of Copenhagen, Copenhagen, Denmark. (e-mail: m.loog@tudelft.nl)

The surrogate loss corresponds to the loss we would try to minimize if we did have labels for the unlabeled objects. Considering the same criterion in the supervised and semi-supervised case aligns the goal of constructing a semi-supervised classifier with the one used when constructing a supervised classifier. By doing this, we avoid conflating improved performance based on a change in surrogate loss function with improvements gained by the availability of unlabeled data. For the same reason we also keep the regularization parameter fixed in objective functions of the supervised and semi-supervised classifiers.

The main conclusion from our analysis (Theorems 1 and 2) is that for classifiers defined by convex margin-based surrogate losses that are monotonically decreasing, it is impossible to come up with *any* semi-supervised approach that is able to guarantee safe improvement. We also consider the case of non-monotonically decreasing losses and in particular explore the case of the quadratic loss. We show under what conditions it *is* possible in this case to come up with a semi-supervised classifier that provides safe improvements over the supervised classifier.

The rest of this work is structured as follows. We start by introducing margin-based loss functions in the empirical risk minimization framework and the extension to the semi-supervised setting. In this, we only treat binary linear classifiers. Though not a real restriction, it does simplify our exposition and allows us to focus on the core ideas. In Section 3, we introduce a strict notion of safe semi-supervised learning. We first show for which class of common loss functions it is impossible to derive any semi-supervised learning strategy that is no worse than the supervised classifier for all possible labelings of the unlabeled data. We then consider the case of soft assignment of unlabeled objects to classes. Here, too, it is impossible to provide a strict improvement guarantee for this class of monotonically decreasing loss functions. We subsequently show for what losses it is possible to get strict improvements and discuss some practical approaches to using this insight. In Section 5 we apply the theory to a few well-known loss functions. In Section 6 we discuss how these results relate to other results on the (im)possibility of semi-supervised learning and what the implications of these results are for approaches to safe semi-supervised learning.

2. PRELIMINARIES

We consider binary linear classifiers in the empirical risk minimization framework. Let \mathbf{X} be an $L \times d$ design matrix of L labeled objects, where each row \mathbf{x}^\top is a d -dimensional vector of feature values corresponding to each labeled object. Let $\mathbf{y} \in \{-1, +1\}^L$ be the corresponding label vector. The vector $\mathbf{w} \in \mathbb{R}^d$ contains the weights defining a linear classifier through $\text{sign}(\mathbf{x}^\top \mathbf{w})$. We consider convex margin-based surrogate loss functions, which are loss functions of the form $\phi(\mathbf{y}\mathbf{x}^\top \mathbf{w})$. Many well-known classifiers can be described in this way, including logistic regression, least squares classification and support vector machines (see also Figure 1).

2.1 Empirical Risk Minimization

In the empirical risk minimization framework a classifier is obtained by minimizing a chosen surrogate loss ϕ over a set of training objects plus an optional

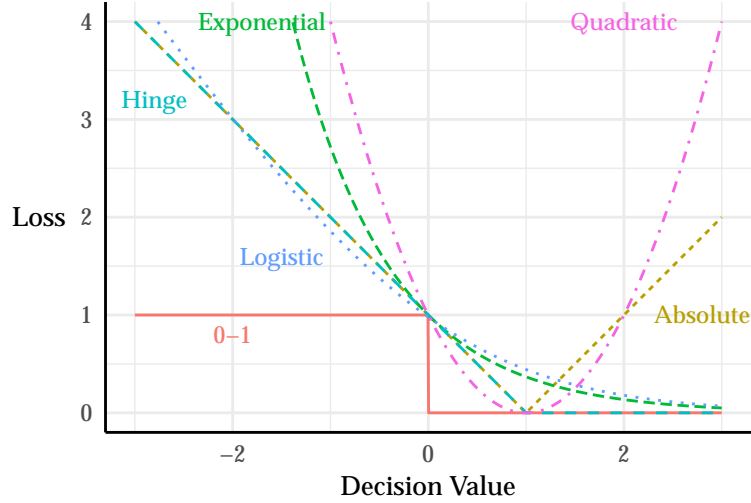


FIG 1. Different Margin-based losses

regularization term Ω , which we take to be a convex function of \mathbf{w} :

$$(1) \quad R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \sum_{i=1}^L \phi(y_i \mathbf{x}_i^\top \mathbf{w}) + \lambda \Omega(\mathbf{w}).$$

By minimizing this with respect to \mathbf{w} we get a supervised classifier:

$$\mathbf{w}_{\text{sup}} = \arg \min_{\mathbf{w}} R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y}).$$

In the semi-supervised setting, we have an additional design matrix corresponding to unlabeled objects \mathbf{X}_u , sized $U \times d$, with unknown labels $\mathbf{y}_u \in \{-1, +1\}^U$. We therefore consider the corresponding semi-supervised risk function:

$$(2) \quad R_\phi^{\text{semi}}(\mathbf{w}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) = R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y}) + \sum_{i=1}^U q_i \phi(\mathbf{x}_i^\top \mathbf{w}) + (1 - q_i) \phi(-\mathbf{x}_i^\top \mathbf{w}),$$

where $\mathbf{q} \in [0, 1]^U$ are what we will refer to as *responsibilities*, indicating the unknown and possibly ‘soft’ membership of each object to a class. For instance, if the true labels were known these would correspond to ‘hard’ responsibilities $\mathbf{q}^{\text{true}} \in \{0, 1\}^U$ and the semi-supervised risk formulation becomes equal to the supervised risk formulation in Equation (1), where the sum is now over the L labeled objects and the U objects for which we did not have a label.

3. LIMITS OF SAFE SEMI-SUPERVISION

Even though we know the true labeling of the unlabeled objects in Equation (2) belongs to some $\mathbf{q} \in \{0, 1\}^U$, we do not know which one. We say that a semi-supervised procedure \mathbf{w}_{semi} is *safe* if it is guaranteed to attain a loss on the

labeled and unlabeled objects equal to or lower than the supervised solution for all possible labelings of the data, since this is guaranteed to include the true labeling of the unlabeled objects. In the remainder of this section we formalize this definition of safety, consider the cases of hard and soft labeling, and come to our negative results: for many loss functions safe semi-supervision is, in fact, not possible.

3.1 Hard labeling

Let D_ϕ denote the difference in terms of the chosen loss ϕ on a set of objects between a new classifier \mathbf{w} and the supervised classifier \mathbf{w}_{sup} for some set of responsibilities for the unlabeled data:

$$D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) = R_\phi^{\text{semi}}(\mathbf{w}_{\text{semi}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) - R_\phi^{\text{semi}}(\mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}).$$

The true unknown labels can in principle correspond to any $\mathbf{q} \in \{0, 1\}^U$. For a semi-supervised classifier \mathbf{w}_{semi} to be guaranteed to be better than the supervised classifier we therefore need that:

$$(3) \quad \max_{\mathbf{q} \in \{0, 1\}^U} D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) \leq 0$$

and the inequality should be strict for at least one instantiation of \mathbf{q} . Is it possible to construct some semi-supervised strategy that has this guaranteed improvement over the supervised solution for margin-based surrogate losses? The following theorem gives a condition under which this strict improvement is never possible.

THEOREM 1. *Let \mathbf{w}_{sup} be a minimizer of $R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y})$ and assume it is unique. If ϕ is a monotonically decreasing convex margin-based loss function, meaning $\phi(a) \geq \phi(b)$ for $a \leq b$, then there is no safe semi-supervised procedure which guarantees Equation (3) while having at least one \mathbf{q}^* for which $D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*) < 0$*

PROOF. We are going to prove this by contradiction. So let us assume that $D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*) < 0$ and define M to be $R_\phi(\mathbf{w}_{\text{semi}}, \mathbf{X}, \mathbf{y}) - R_\phi(\mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y})$. The latter is the difference in surrogate loss between the supervised and semi-supervised learner on the labeled data. Based on our assumption we can now write

$$\begin{aligned} M + \sum_{i=1}^U q_i^* \phi(\mathbf{x}_i^\top \mathbf{w}_{\text{semi}}) + (1 - q_i^*) \phi(-\mathbf{x}_i^\top \mathbf{w}_{\text{semi}}) \\ - \sum_{i=1}^U q_i^* \phi(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) - (1 - q_i^*) \phi(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) < 0. \end{aligned}$$

$M > 0$ since \mathbf{w}_{sup} is the unique minimizer of $R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y})$. Thus

$$\begin{aligned} \sum_{i=1}^U q_i^* \phi(\mathbf{x}_i^\top \mathbf{w}_{\text{semi}}) + (1 - q_i^*) \phi(-\mathbf{x}_i^\top \mathbf{w}_{\text{semi}}) \\ < \sum_{i=1}^U q_i^* \phi(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) + (1 - q_i^*) \phi(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}). \end{aligned}$$

Now consider the set of indices $i \in \mathcal{I}$ of all objects for which the loss of the semi-supervised solution is lower than the loss of the supervised solution, given the responsibility \mathbf{q}^* , i.e.,

$$\begin{aligned} & q_i^* \phi(\mathbf{x}^\top \mathbf{w}_{\text{semi}}) + (1 - q_i^*) \phi(-\mathbf{x}^\top \mathbf{w}_{\text{semi}}) \\ & < q_i^* \phi(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + (1 - q_i^*) \phi(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}). \end{aligned}$$

\mathcal{I} is not empty, because by construction the total loss on the unlabeled objects for responsibility \mathbf{q}^* is lower for \mathbf{w}_{semi} than for \mathbf{w}_{sup} . For each $i \in \mathcal{I}$, either $q_i^* = 1$ or $q_i^* = 0$. If $q_i^* = 1$, $\phi(\mathbf{x}^\top \mathbf{w}_{\text{semi}}) < \phi(\mathbf{x}^\top \mathbf{w}_{\text{sup}})$. Because ϕ is monotonically decreasing, it holds that $\mathbf{x}^\top \mathbf{w}_{\text{semi}} > \mathbf{x}^\top \mathbf{w}_{\text{sup}}$. We also have $-\mathbf{x}^\top \mathbf{w}_{\text{semi}} < -\mathbf{x}^\top \mathbf{w}_{\text{sup}}$ and because ϕ is monotonically decreasing $\phi(-\mathbf{x}^\top \mathbf{w}_{\text{semi}}) \geq \phi(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})$. So changing label from $q_i^* = 1$ to $q_i^{\text{new}} = 0$, the inequality is reversed. If $q_i^* = 0$, using the same argument, the inequality is also reversed if we choose $q_i^{\text{new}} = 1$ for these objects. This gives us

$$\begin{aligned} & q_i^{\text{new}} \phi(\mathbf{x}^\top \mathbf{w}_{\text{semi}}) + (1 - q_i^{\text{new}}) \phi(-\mathbf{x}^\top \mathbf{w}_{\text{semi}}) \\ & \geq q_i^{\text{new}} \phi(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + (1 - q_i^{\text{new}}) \phi(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}) \end{aligned}$$

for each $i \in \mathcal{I}$. Since $i \in \mathcal{I}$ are the only objects for which the loss on the unlabeled objects decreased for the semi-supervised classifier compared and if we let $q_i^{\text{new}} = q_i^*$ for $i \notin \mathcal{I}$ we have

$$D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^{\text{new}}) > 0.$$

which contradicts Equation (3). \square

REMARK 1. *Alternatively, we can drop the requirement that \mathbf{w}_{sup} is the unique minimizer of $R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y})$ by requiring the loss functions to be strictly decreasing.*

3.2 Beyond Hard Labelings

In Equation (3) we considered improvement over all hard labelings of the unlabeled data. Alternatively we could also consider improvements for the larger set of all soft assignments of labels to classes, meaning

$$(4) \quad \max_{\mathbf{q} \in [0,1]^U} D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) \leq 0$$

and at least one $\mathbf{q} \in [0,1]^U$ for which the inequality is strict. There are several reasons why this is an interesting relaxation to consider. First of all it requires the semi-supervised solution to guarantee improvements for a larger class of responsibilities than just the hard labelings, meaning it becomes more difficult to construct a procedure with this property. If a procedure guarantees improvement in this sense, it implies it also works for all possible hard labelings. Secondly, it corresponds to a scenario different from the hard labeling where there is uncertainty in the labels of the unlabeled objects. And lastly, the convex constraint makes the problem more amenable to analysis and is, in fact, used by approaches such as MCPL [8] and ICLS [9].

The set of classifiers given by all different responsibilities turns out to be a useful concept.

DEFINITION 1. The constraint set \mathcal{C}_ϕ is the set of all possible classifiers that can be obtained by minimizing the semi-supervised loss for any vector of responsibilities \mathbf{q} assigned to the unlabeled data, i.e.,

$$\mathcal{C}_\phi = \left\{ \arg \min_{\mathbf{w}} R_\phi^{\text{semi}}(\mathbf{w}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}) \mid \mathbf{q} \in [0, 1]^U \right\}.$$

The following lemma provides an intermediary step towards our second negative result. It tells us that no strict improvement is possible if the supervised solution is already part of the constraint set.

LEMMA 1. If $R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y})$ is strictly convex and $\mathbf{w}_{\text{sup}} \in \mathcal{C}_\phi$, then there is a soft assignment \mathbf{q}^* such that for every choice of semi-supervised classifier $\mathbf{w}_{\text{semi}} \neq \mathbf{w}_{\text{sup}}$, $D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*) > 0$.

PROOF. As $\mathbf{w}_{\text{sup}} \in \mathcal{C}_\phi$ there is a soft labeling \mathbf{q}^* such that \mathbf{w}_{sup} minimizes the semi-supervised risk $R_\phi^{\text{semi}}(\mathbf{w}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*)$. This risk function is strictly convex because the supervised risk is strictly convex and therefore \mathbf{w}_{sup} is its unique minimizer. This immediately implies that for every $\mathbf{w}_{\text{semi}} \neq \mathbf{w}_{\text{sup}}$, we have that $R_\phi^{\text{semi}}(\mathbf{w}_{\text{semi}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*) > R_\phi^{\text{semi}}(\mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*)$. \square

REMARK 2. The requirement to have a strictly convex supervised risk function can be relaxed. What we basically need in the proof is that \mathbf{w}_{sup} is the unique optimizer for $R_\phi^{\text{semi}}(\mathbf{w}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*)$. Nevertheless, unlike, for instance, a hinge loss that is not regularized by something like a 2-norm of the weight vector, many interesting objective functions are strictly convex.

For monotonically decreasing margin-based losses, we now show that we can always explicitly construct a \mathbf{q}^* , such that the corresponding semi-supervised solution equals the original supervised one. With this, a result similar to Theorem 1 for the soft-assignment guarantee directly follows, but first we formulate that explicit construction of the necessary soft labeling.

LEMMA 2. If ϕ is a monotonically decreasing margin-based loss function where for each unlabeled object \mathbf{x} , $\phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})$ and $\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}})$ exist, we can recover \mathbf{w}_{sup} by minimizing the semi-supervised loss by assigning responsibilities $\mathbf{q} \in [0, 1]^U$ as follows:

$$(5) \quad q = \frac{\phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}{\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}$$

PROOF. Consider the case where we have one unlabeled object \mathbf{x} with responsibility q . The semi-supervised objective then becomes

$$R_\phi^{\text{semi}}(\mathbf{w}) = R_\phi^{\text{sup}}(\mathbf{w}, \mathbf{X}, \mathbf{y}) + q\phi(\mathbf{x}^\top \mathbf{w}) + (1 - q)\phi(-\mathbf{x}^\top \mathbf{w}).$$

We need to find a $q \in [0, 1]$ that causes the gradient of this objective, evaluated in the supervised solution, to remain equal to zero:

$$(6) \quad \begin{aligned} \nabla_{\mathbf{w}} R_\phi^{\text{semi}}(\mathbf{w}_{\text{sup}}) &= \mathbf{0} + q\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}})\mathbf{x} \\ &\quad - (1 - q)\phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})\mathbf{x} \\ &= \mathbf{0} \end{aligned}$$

where ϕ' denotes the derivative of $\phi(a)$ with respect to a . As long as $\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}) \neq 0$, we can explicitly solve for q to get

$$(7) \quad q = \frac{\phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}{\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}.$$

If ϕ is a monotonically decreasing loss, then

$$\phi'(a) \leq 0$$

and for each object $0 \leq q \leq 1$. Since this can be done for each object individually, we can do it for all objects to get a vector of responsibilities $\mathbf{q} \in [0, 1]^U$. \square

Now that we have shown by a constructive argument that for monotonically decreasing margin-based losses it always holds that $\mathbf{w}_{\text{sup}} \in \mathcal{C}_\phi$, the following result is straightforward.

THEOREM 2. *Let ϕ be a monotonically decreasing convex margin-based loss function and \mathbf{w}_{sup} be the unique minimizer of $R_\phi(\mathbf{w}, \mathbf{X}, \mathbf{y})$. There is no semi-supervised classifier \mathbf{w}_{semi} for which Equation (4) holds, while having at least one \mathbf{q}^* for which $D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*) < 0$.*

PROOF. This follows directly from Lemma 1 and Lemma 2. \square

This means that for monotonically decreasing loss functions it is impossible to construct a semi-supervised learner that, in terms of its surrogate loss on the full training data, is never outperformed by the supervised solution. In other words, if the semi-supervised classifier is taken to be different from the supervised classifier, there is always the risk that there is a true labeling of the unlabeled data for which the loss of the semi-supervised learner on the full data becomes larger than the loss of the supervised one.

Is it unexpected that semi-supervised learning cannot be done safely in this setting? For whom it is not, it may then come as a surprise that there are margin-based losses for which it is actually possible to construct safe semi-supervised learners.

4. POSSIBILITIES FOR SAFE SSL

If we look beyond the previous losses, and consider non-monotonically decreasing ones, we may still be able to get a classifier that is guaranteed to be better than the supervised solution in terms of the surrogate loss, even in the pessimistic regime. When can we expect strict safe semi-supervised learning to allow for improvements of its supervised counterpart? And if improvements are possible, how then do we construct an actual classifier that does so in a safe way?

To construct a semi-supervised learner that at least is guaranteed to never be worse, we need to find that \mathbf{w} that minimizes $D_\phi(\mathbf{w}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q})$ for all possible \mathbf{q} . This corresponds, more precisely, to the following minimax problem:

$$(8) \quad \max_{\mathbf{q} \in [0, 1]^U} \min_{\mathbf{w}} D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}).$$

This is a formulation similar to the one used in [8], where instead of margin-based losses, the loss functions are log-likelihoods of a generative model. Similar to [8], it is clear that Equation (8) can never be larger than 0. This simply indicates that we can always find a semi-supervised learner that is at least as good as the supervised one. To show that we can do better than that, consider the following.

If R_ϕ^{semi} is convex in \mathbf{w} , then since the objective is linear in \mathbf{q} and $[0, 1]^U$ is a compact space we can invoke [10, Corollary 3.3], allowing us to interchange the maximization and the minimization, which in turn implies that there is a solution to the above which is a saddle point $(\mathbf{w}_{\text{semi}}, \mathbf{q}^*)$ to the objective function. Assume the function

$$\max_{\mathbf{q} \in [0, 1]^U} D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q})$$

is strictly convex in \mathbf{w} (this is the case for instance if D_ϕ is strictly convex for every fixed \mathbf{q} [11, Chapter 8]), then the solution \mathbf{w}_{semi} is unique. The vector \mathbf{w}_{semi} is the minimizer of D_ϕ and therefore of R_ϕ^{semi} . Because $(\mathbf{w}_{\text{semi}}, \mathbf{q}^*)$ is a saddle point, \mathbf{q}^* provides the responsibilities that lead to this minimizer and therefore \mathbf{w}_{semi} is in \mathcal{C}_ϕ .

Now if \mathbf{w}_{sup} is not in \mathcal{C}_ϕ , then $\mathbf{w}_{\text{sup}} \neq \mathbf{w}_{\text{semi}}$ and so $D_\phi(\mathbf{w}_{\text{semi}}, \mathbf{w}_{\text{sup}}, \mathbf{X}, \mathbf{y}, \mathbf{X}_u, \mathbf{q}^*)$ must be strictly smaller than 0, because of the strict convexity of the loss. This means that for the worst case responsibilities, \mathbf{w}_{semi} would strictly improve upon \mathbf{w}_{sup} and, by the property of a saddle point, whatever the true responsibilities are, at least as large an improvement can be expected.

4.1 Some Sufficient Conditions

So all that is required to show that the procedure just described leads to an improved classifier is therefore that $\mathbf{w}_{\text{sup}} \notin \mathcal{C}_\phi$. For an unlabeled data set consisting of a single sample \mathbf{x} , this is readily done by reconsidering the proof of Lemma 2. In particular, rewriting Equation (6), we can conclude the following:

LEMMA 3. *If for $\mathbf{X}_u = \mathbf{x}^\top$ there is no $q \in [0, 1]$ such that*

$$(\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}))\mathbf{x}q = (\phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}))\mathbf{x}$$

then $\mathbf{w}_{\text{sup}} \notin \mathcal{C}_\phi$ so \mathbf{w}_{semi} has to be different from \mathbf{w}_{sup} and, therefore, the former has to improve over the latter.

The case in which $U > 1$ turns out to be hard to fully characterize. Again starting from Equation (6), we can state that if there is no \mathbf{q} such that

$$\sum_{i=1}^U q_i \phi'(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}})\mathbf{x}_i - (1 - q_i) \phi'(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}})\mathbf{x}_i = \mathbf{0}$$

then the gradient evaluated in the supervised solution of the objective function over all training data is not zero and so the semi-supervised solution is different, therefore improving over the supervised solution. But this result is hardly insightful. For one, it is unclear if this at all happens when $U > 1$. We do, however, have a sufficient condition that leads the semi-supervised learner to improve over the supervised counterpart. For this, we consider convex, margin-based losses ϕ that are decreasing left of 1 and right of 1 start to increase monotonically, as for instance, in the cases of the quadratic or absolute loss. So these

losses also increasingly penalize overestimation of the label value of every object.

THEOREM 3. *Let*

$$\phi'(a) \begin{cases} \leq 0, & \text{if } a \leq 1 \\ > 0, & \text{if } a > 1. \end{cases}$$

If, for all $\mathbf{x} \in X_u$, $|\mathbf{x}^\top \mathbf{w}_{\text{sup}}|$ is larger than 1, then $\mathbf{w}_{\text{semi}} \neq \mathbf{w}_{\text{sup}}$. That is, we get an improved semi-supervised estimator if all points in X_u are outside of the margin.

PROOF. Without loss of generality, we can assume that we have translated, rotated, and scaled our data such that the supervised solution is given by $\mathbf{w}_{\text{sup}} = (1, 0, \dots, 0)^\top$. Such standardization of the data does not lead to an essentially different problem.

It is easy to check that for every $\mathbf{x}^\top \mathbf{w}_{\text{sup}} = x_{i1} > 1$, we have $\phi'(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) = \phi'(x_{i1}) > 0$, where x_{i1} indicates the first coordinate of sample \mathbf{x}_i . Likewise, we have $\phi'(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) = \phi'(-x_{i1}) < 0$. It therefore follows, for every choice of $q_i \in [0, 1]$, that $q_i \phi'(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) x_{i1} - (1 - q_i) \phi'(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) x_{i1} > 0$. Likewise, for every $\mathbf{x}^\top \mathbf{w}_{\text{sup}} = x_{i1} < 1$, we have the same result: for every choice of $q_i \in [0, 1]$, $q_i \phi'(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) x_{i1} - (1 - q_i) \phi'(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) x_{i1} > 0$. This shows that the first equation in the system given by

$$\sum_{i=1}^U q_i \phi'(\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) \mathbf{x}_i - (1 - q_i) \phi'(-\mathbf{x}_i^\top \mathbf{w}_{\text{sup}}) \mathbf{x}_i = \mathbf{0}$$

does not equal 0, and so the gradient differs from zero, meaning that the supervised solution cannot be the optimal one. \square

The restriction that all points should be outside of the margin is, of course, rather strong. But, as indicated, the requirement is only sufficient and certainly not necessary. Subsection 5.3 gives an additional result for the squared loss.

4.2 Methods for Pessimistic SSL

The idea of using the constraint space to construct a semi-supervised learner has been operationalized in two ways. In implicitly constrained semi-supervised learning [9], one minimizes a supervised loss function on the L labeled objects, under the constraint that this solution has to be the loss minimizer on all of the data, for a particular (partial) labeling of the data:

$$\min_{\mathbf{w} \in \mathcal{C}_\phi} R_\phi(\mathbf{w})$$

with \mathcal{C}_ϕ as in Definition 1. If $\mathbf{w}_{\text{sup}} \in \mathcal{C}_\phi$, this approach will not update the supervised classifier. Only if $\mathbf{w}_{\text{sup}} \notin \mathcal{C}_\phi$ will the implicitly constrained solution be different from the supervised alternative.

A related but different approach is to enforce the non-degradation guarantee by using Equation (8) directly [8]. This is referred to as a pessimistic and contrastive objective, where the pessimism refers to considering all possible labelings, and the contrast refers to the fact that the loss of the semi-supervised solution is compared to the loss of the supervised solution.

TABLE 1
Margin-based loss functions and their corresponding responsibilities

Name	$\phi(y\mathbf{x}^\top \mathbf{w}_{\text{sup}})$	$q(\mathbf{x}^\top \mathbf{w}_{\text{sup}})$	Range
Logistic	$\sqrt{2} \log(1 + \exp(-y\mathbf{x}^\top \mathbf{w}_{\text{sup}}))$	$(1 + \exp(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}))^{-1}$	$(0, 1)$
Quadratic	$(1 - y\mathbf{x}^\top \mathbf{w}_{\text{sup}})^2$	$\frac{1}{2}(\mathbf{x}^\top \mathbf{w}_{\text{sup}} + 1)$	$(-\infty, \infty)$
Hinge	$\max(1 - y\mathbf{x}^\top \mathbf{w}_{\text{sup}}, 0)$	$\begin{cases} \frac{1}{2}, & \text{if } -1 < \mathbf{x}^\top \mathbf{w}_{\text{sup}} < 1 \\ 1, & \text{if } \mathbf{x}^\top \mathbf{w}_{\text{sup}} > 1 \\ 0 & \text{if } \mathbf{x}^\top \mathbf{w}_{\text{sup}} < -1 \end{cases}$	$\{0, \frac{1}{2}, 1\}$
Exponential	$\exp(-y\mathbf{x}^\top \mathbf{w}_{\text{sup}})$	$\exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}})(\exp(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}}))^{-1}$	$(0, 1)$
Absolute	$ 1 - y\mathbf{x}^\top \mathbf{w} $	$\begin{cases} \frac{1}{2}, & \text{if } -1 < y\mathbf{x}^\top \mathbf{w}_{\text{sup}} < 1 \\ \text{No solution,} & \text{otherwise} \end{cases}$	$\{\frac{1}{2}\}$

Thus, in both implicitly constrained and contrastive pessimistic learning, the minimization only leads to a solution different from \mathbf{w}_{sup} if $\mathbf{w}_{\text{sup}} \notin \mathcal{C}_\phi$. In both cases there are theorems stating that, under certain conditions, if the resulting classifier is different from the supervised solution, it improves over the supervised alternative.

5. EXAMPLES

We will consider both some examples of monotonically decreasing losses and a non-monotonically decreasing loss. In the first case we will show how the (partial) labels can always be set to reconstruct the supervised solution. In the second case we will show why for some losses it is not possible to set the responsibilities in such a way as to recover the supervised solution. The results are summarized in Table 1.

5.1 Logistic Loss

Consider the logistic loss function given by

$$\phi(y\mathbf{x}^\top \mathbf{w}) = \log(1 + \exp(-y\mathbf{x}^\top \mathbf{w}))$$

and whose minimization leads to the logistic regression classifier. Its derivative is given by

$$\phi'(y\mathbf{x}^\top \mathbf{w}) = \frac{-\exp(-y\mathbf{x}^\top \mathbf{w})}{1 + \exp(-y\mathbf{x}^\top \mathbf{w})}$$

from which we can verify it is a monotonically decreasing loss. Applying Equation (5) we find that

$$(9) \quad q = \frac{-\exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}})}{1 + \exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}})} \times \left(\frac{-\exp(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}{1 + \exp(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})} + \frac{-\exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}})}{1 + \exp(\mathbf{x}^\top \mathbf{w}_{\text{sup}})} \right)^{-1}.$$

Because the second term equals -1 , after rewriting the first term, we have

$$q = \frac{1}{1 + \exp(-\mathbf{x}^\top \mathbf{w}_{\text{sup}})}.$$

This is equal to the class posterior of the positive class, given by the logistic regression model. Thus we see that the responsibility assigned to the new object is exactly the class posterior assigned by logistic regression.

5.2 Support Vector Machine

The hinge loss, employed in support vector classification, has the form

$$\phi(y\mathbf{x}^\top \mathbf{w}) = \max(1 - y\mathbf{x}^\top \mathbf{w}, 0).$$

The value for the derivative at all points except $1 - y\mathbf{x}^\top \mathbf{w} = 0$ is given by

$$\phi'(y\mathbf{x}^\top \mathbf{w}) = \begin{cases} -1, & \text{if } 1 - y\mathbf{x}^\top \mathbf{w} > 0 \\ 0, & \text{otherwise.} \end{cases}$$

Plugging this into Equation (5), we have that

$$q = \begin{cases} \frac{1}{2}, & \text{if } -1 < \mathbf{x}^\top \mathbf{w}_{\text{sup}} < 1 \\ 1, & \text{if } \mathbf{x}^\top \mathbf{w}_{\text{sup}} > 1 \\ 0 & \text{if } \mathbf{x}^\top \mathbf{w}_{\text{sup}} < -1. \end{cases}$$

If the prediction is strongly positive (respectively, negative), it will be assigned to the positive (negative) class. If on the other hand, it is within the margin, it gets assigned to both classes equally. It means for the unlabeled objects in the margin, any change in $\mathbf{x}^\top \mathbf{w}_{\text{sup}}$ has an opposite contribution for the part of the loss corresponding to the positive and the negative class. Only by weighting the two options equally will a change in $\mathbf{x}^\top \mathbf{w}_{\text{sup}}$ not yield a change in the loss.

5.3 Quadratic Loss

Now consider the quadratic loss, which is a non-monotonically decreasing loss function:

$$\phi(y\mathbf{x}^\top \mathbf{w}) = (1 - y\mathbf{x}^\top \mathbf{w})^2.$$

Its derivative is

$$\phi'(y\mathbf{x}^\top \mathbf{w}) = -2(1 - y\mathbf{x}^\top \mathbf{w}).$$

Again using (5) we find that

$$q = \frac{-2(1 + \mathbf{x}^\top \mathbf{w}_{\text{sup}})}{-2(1 - \mathbf{x}^\top \mathbf{w}_{\text{sup}}) - 2(1 + \mathbf{x}^\top \mathbf{w}_{\text{sup}})}$$

which we can simplify to

$$q = \frac{\mathbf{x}^\top \mathbf{w}_{\text{sup}} + 1}{2}.$$

This is the rescaling of the decision function from the interval $[-1, +1]$ to $[0, 1]$. Note that in this case $\mathbf{x}^\top \mathbf{w}$ is not necessarily restricted to be within $[-1, +1]$ and so it may occur that $q \notin [0, 1]$. In this case there is no assignment of the responsibilities that recovers the supervised solution and thus the unlabeled data forces us to update the decision function $\mathbf{x}^\top \mathbf{w}$.

When $U > 1$, for the monotonically decreasing loss functions, it was enough to show that each $q_i \in [0, 1]$ can be set individually in order to reconstruct the supervised solution using a responsibility vector $\mathbf{q} \in [0, 1]^U$. For the quadratic loss, however, the situation is more complex when multiple unlabeled objects are available. This is because, considering each q_i individually might not allow us to find $\mathbf{q} \in [0, 1]^U$ for which the gradient of the semi-supervised objective

at the supervised solution is equal to zero, but there could still be a combined $\mathbf{q} \in [0, 1]^U$ for which this does hold, as we discussed for the general case in Theorem 3.

It turns out that if the dimensionality $d \geq U$, such a $\mathbf{q} \in [0, 1]^U$ does not exist as long as

$$\mathbf{X}_u \mathbf{w}_{\text{sup}} \notin [-1, 1]^U.$$

The proof of this is in the appendix but is basically a restatement of the Theorem 3. If $d \leq U$, however, then it is also guaranteed that such $\mathbf{q} \in [0, 1]^U$ does not exist if

$$\|\mathbf{X}_u \mathbf{w}_{\text{sup}}\|_2 > \sqrt{U}.$$

This last results is essentially different from Theorem 3 as it shows that even if some of the unlabeled points are within the margin, the semi-supervised learner has to be different from the supervised if one or more of the unlabeled points are sufficiently far outside of the margin.

5.4 Absolute Loss

The absolute loss is given by

$$\phi(y\mathbf{x}^\top \mathbf{w}) = |1 - y\mathbf{x}^\top \mathbf{w}|.$$

and its derivative at all values except $1 - y\mathbf{x}^\top \mathbf{w} = 0$ then becomes

$$\phi'(y\mathbf{x}^\top \mathbf{w}) = \begin{cases} -1, & \text{if } 1 - y\mathbf{x}^\top \mathbf{w} > 0 \\ +1, & \text{otherwise.} \end{cases}$$

When $-1 < y\mathbf{x}^\top \mathbf{w}_{\text{sup}} < 1$, we can use Equation (5) to find $q = \frac{1}{2}$. Otherwise, $\phi'(\mathbf{x}^\top \mathbf{w}_{\text{sup}}) + \phi'(-\mathbf{x}^\top \mathbf{w}_{\text{sup}}) = 0$ and there is no q that makes the gradient of the semi-supervised objective in the supervised solution equal to zero. In that case, when we have a single unlabeled object, the semi-supervised solution is an improvement over the supervised solution. For the case of multiple unlabeled objects it may again be possible to find a vector of responsibilities $\mathbf{q} \in [0, 1]^U$ that recovers the supervised solution. Again, Theorem 3 offers a sufficient condition where the semi-supervised solution must improve over its supervised counterpart.

6. DISCUSSION

6.1 Impossibilities of Semi-supervised Learning

As [12] and others have argued, for diagnostic methods, where $p(y|\mathbf{x})$ gets modeled directly and not through modeling the joint distribution $p(y, \mathbf{x})$, semi-supervised learning without additional assumptions should be impossible because the parameters of $p_{Y|X}$ and p_X are a priori independent. Considering why they do not allow for safe semi-supervised versions offers a different understanding of why this may or may not be true. While our results applied to logistic regression corroborates their claim, the quadratic loss shows a counter example. This shows that for non-monotonically decreasing losses, even safe improvements are possible in the diagnostic setting. One important difference in our analysis is that we consider the minimization of a loss function that may not

induce a correct probability. It is the monotonic decreasingness of the loss, rather than correspondence to a probabilistic model that determines whether safe semi-supervised learning is possible. Moreover, some of the losses for which semi-supervised learning is possible are successfully applied in supervised learning in practice and it is therefore interesting that safe semi-supervised versions exist.

It has also been suggested that the possibility of semi-supervised learning depends on the causal direction of $p_{Y|X}$ [13]. This seems at odds with our result that pessimistic semi-supervised learning is possible for non-monotonically decreasing losses, regardless of the causal structure of the problem. We think this is again due to the our lack of assumptions that the model that is used is a correctly specified probabilistic model, which is required for the results in [13] to hold.

Our results also might seem to contradict the result by [14] that, when the supervised model is misspecified, a particular semi-supervised adaptation of logistic regression has an asymptotic variance that is at least as small as supervised logistic regression. In this work, however, we cover the pessimistic setting where a semi-supervised learner needs to outperform the supervised learner for all possible labelings in a finite sample setting. This is a much stricter requirement than the asymptotic result in [14]. Moreover, we do not require the supervised model to be misspecified. For semi-supervised learning in general, their result is encouraging, while for safe semi-supervised learning it makes sense to consider the results in the pessimistic setting.

6.2 Safe semi-supervised learning

What do our results mean for ‘safe’ approaches to semi-supervised learning, such as those proposed in [15] and [16]? The results in [16] show their proposed procedure is asymptotically safe, similar to the results in [14], but under weaker assumptions. In our analysis, we consider performance on the limited set of labeled and unlabeled objects. For monotonically decreasing margin-based losses, it may still be possible to find a procedure that outperforms supervised learning in expectation, but not on a particular set of objects for all its labelings.

The improvement guarantee, in terms of classification accuracy, of the safe semi-supervised SVM by [15] depends on the assumption that the true labeling of the objects is given by one of the low-density separators that their algorithm finds. An advantage of our analysis is that we avoid making such untestable assumptions. The consequence of this is that all possible labelings are considered, not just those corresponding to a low-density separator. If their low-density assumptions holds, their method provides one way of making use of this information. As we have demonstrated, however, in a worst case sense no such guarantees can be given, at least in terms of the semi-supervised objective considered in our work. Without making these untestable assumptions, our results show a safe semi-supervised support vector machine is impossible.

6.3 Consequences and Opportunities

The results of Theorem 1 and Theorem 2 show that for many well-known losses that are monotonically decreasing, it is impossible to construct a safe semi-supervised method that is guaranteed to not lead to worse performance than the supervised solution, without making additional assumptions. In this way, these

results offer a different perspective on why this type of semi-supervised learning is not possible for some losses, by indicating the monotonic decreasingness property as essential to the proofs.

One consequence of these results is that if we want to construct semi-supervised learners with the type of guarantee studied here, we need more constraints than those given by the pessimistic approach, to reduce the size of the set of possible label assignments that is considered. For unlabeled data to be helpful, we need additional constraints on the semi-supervised solution coming from substantive assumptions, like a low-density or clustering assumption. We need to keep in mind that these strong assumptions, however, might have also helped improve the supervised solution, without considering the unlabeled data, and properly compare any improvements of the semi-supervised learner to a supervised learner that also takes these assumptions into account.

We have also shown that for the non-monotonically decreasing loss functions, safe improvement is possible. One could ascribe this fact to a peculiar property of these losses: they give increasingly higher loss even if the sign of the decision function is correct. The improvements in terms of the loss that we get may therefore not be useful for classification, since they may be in a part of the loss function where the surrogate loss already forms a bad approximation to the $\{0, 1\}$ -loss. In the supervised case, however, surrogate losses like the quadratic loss generally give decent performance in terms of the error rate. In some sense it is therefore not surprising that its pessimistic semi-supervised counterpart has also shown increased performance as more unlabeled data is added to the training set [9].

Our analysis takes a rather extreme view of what is required to be safe, where the semi-supervised learner has to outperform the supervised learner on every possible dataset. A less strict notion of safety might consider this improvement to hold in expectation over datasets or labelings, rather than for a particular dataset. On any one particular dataset that a practitioner is faced with, however, the unlabeled data may then cause a decrease in the performance compared to the supervised classifier.

7. CONCLUSION

We have shown that for the class of convex margin-based losses, the fact whether they are monotonically decreasing or not plays a key role in whether they admit safe semi-supervised procedures. In particular, we have shown that, without making additional assumptions, it is impossible to construct safe semi-supervised procedures for monotonically decreasing losses by showing what partial assignment of the unlabeled objects leads to the recovery of the supervised classifier from a semi-supervised objective. This subsequently implied that if we choose any semi-supervised procedure that deviates from the supervised solution, there is some labeling of the unlabeled objects (which could be the true labeling) for which it decreases performance. While this means that for many supervised procedures it is impossible to construct a safe semi-supervised learner in this strict sense, some losses do admit such solutions. A less strict guarantee might admit performance improvement by aiming for semi-supervised solutions that in expectation rather than on any particular dataset, outperform their supervised counterparts.

The stark reality is that if one sticks to safe semi-supervised learning, beside opportunities for some surrogate losses, there are clear limits to the development of such procedures. It is this reality that we have characterized.

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APPENDIX A: MULTIPLE OBJECTS FOR THE QUADRATIC LOSS

Whether it is possible to find some \mathbf{q} for which minimizing the semi-supervised objective gives the supervised solution in case of the quadratic loss comes down to the question whether the system of equations

$$(10) \quad \mathbf{X}_u^\top \mathbf{q} = \frac{1}{2}(\mathbf{X}_u^\top \mathbf{1} + \mathbf{X}_u^\top \mathbf{X}_u \mathbf{w}_{\text{sup}})$$

has a solution $\mathbf{q} \in [0, 1]^U$. Let $(\mathbf{X}_u^\top)^+$ denote the Moore-Penrose pseudo-inverse of \mathbf{X}_u^\top . We consider two scenarios: $d \geq U$, the number of unlabeled objects is smaller or equal to the dimensionality of the feature vectors, and $d \leq U$, where we have more unlabeled objects than dimensions.

If $d \geq U$, the pseudo-inverse can be written as $(\mathbf{X}_u \mathbf{X}_u^\top)^{-1} \mathbf{X}_u$ meaning we have a unique solution

$$\mathbf{q} = \frac{1}{2}(\mathbf{1} + \mathbf{X}_u \mathbf{w}_{\text{sup}})$$

and so the supervised solution cannot be recovered unless $\mathbf{X}_u \mathbf{w}_{\text{sup}} \in [-1, 1]^U$.

If $d \leq U$, the pseudo-inverse can be written as $(\mathbf{X}_u^\top)^+ = \mathbf{X}_u (\mathbf{X}_u^\top \mathbf{X}_u)^{-1}$. Rewriting Equation (10) in terms of $\mathbf{r} = 2\mathbf{q} - \mathbf{1}$, the condition for improvement is that

$$\mathbf{X}_u^\top \mathbf{r} = \mathbf{X}_u^\top \mathbf{X}_u \mathbf{w}_{\text{sup}}$$

has no solution $\mathbf{r} \in [-1, 1]^U$. Solving this using the pseudo-inverse we find the solution \mathbf{r}^+ with the smallest norm among all possible solutions:

$$\mathbf{r}^+ = \mathbf{X}_u \mathbf{w}_{\text{sup}}.$$

We therefore have for any solution \mathbf{r} that

$$\|\mathbf{r}\|_2 \geq \|\mathbf{X}_u \mathbf{w}_{\text{sup}}\|_2$$

and so if $\|\mathbf{X}_u \mathbf{w}_{\text{sup}}\|_2 > \sqrt{U}$, this implies that every solution \mathbf{r} lies outside of the unit cube $[-1, 1]^U$ and no proper solution of responsibilities exists.

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